

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSSPTA1623PAZ

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * Welcome to STN International * * * * *

| | | | |
|--------------|----|--------|--|
| NEWS | 1 | | Web Page URLs for STN Seminar Schedule - N. America |
| NEWS | 2 | | "Ask CAS" for self-help around the clock |
| NEWS | 3 | FEB 28 | PATDPAFULL - New display fields provide for legal status data from INPADO |
| NEWS | 4 | FEB 28 | BABS - Current-awareness alerts (SDIs) available |
| NEWS | 5 | MAR 02 | GBFULL: New full-text patent database on STN |
| NEWS | 6 | MAR 03 | REGISTRY/ZREGISTRY - Sequence annotations enhanced |
| NEWS | 7 | MAR 03 | MEDLINE file segment of TOXCENTER reloaded |
| NEWS | 8 | MAR 22 | KOREAPAT now updated monthly; patent information enhanced |
| NEWS | 9 | MAR 22 | Original IDE display format returns to REGISTRY/ZREGISTRY |
| NEWS | 10 | MAR 22 | PATDPASPC - New patent database available |
| NEWS | 11 | MAR 22 | REGISTRY/ZREGISTRY enhanced with experimental property tags |
| NEWS | 12 | APR 04 | EPFULL enhanced with additional patent information and new fields |
| NEWS | 13 | APR 04 | EMBASE - Database reloaded and enhanced |
| NEWS | 14 | APR 18 | New CAS Information Use Policies available online |
| NEWS | 15 | APR 25 | Patent searching, including current-awareness alerts (SDIs), based on application date in CA/CAPLUS and USPATFULL/USPAT2 may be affected by a change in filing date for U.S. applications. |
| NEWS | 16 | APR 28 | Improved searching of U.S. Patent Classifications for U.S. patent records in CA/CAPLUS |
| NEWS | 17 | MAY 23 | GBFULL enhanced with patent drawing images |
| NEWS | 18 | MAY 23 | REGISTRY has been enhanced with source information from CHEMCATS |
| NEWS | 19 | JUN 06 | The Analysis Edition of STN Express with Discover! (Version 8.0 for Windows) now available |
| NEWS | 20 | JUN 13 | RUSSIAPAT: New full-text patent database on STN |
| NEWS | 21 | JUN 13 | FRFULL enhanced with patent drawing images |
| NEWS | 22 | JUN 27 | MARPAT displays enhanced with expanded G-group definitions and text labels |
| NEWS | 23 | JUL 01 | MEDICONF removed from STN |
| NEWS | 24 | JUL 07 | STN Patent Forums to be held in July 2005 |
| NEWS | 25 | JUL 13 | SCISEARCH reloaded |
| NEWS | 26 | JUL 20 | Powerful new interactive analysis and visualization software, STN AnaVist, now available |
| NEWS | 27 | AUG 11 | Derwent World Patents Index(R) web-based training during August |
| NEWS | 28 | AUG 11 | STN AnaVist workshops to be held in North America |
| NEWS EXPRESS | | | JUNE 13 CURRENT WINDOWS VERSION IS V8.0, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 13 JUNE 2005 |
| NEWS HOURS | | | STN Operating Hours Plus Help Desk Availability |
| NEWS INTER | | | General Internet Information |
| NEWS LOGIN | | | Welcome Banner and News Items |
| NEWS PHONE | | | Direct Dial and Telecommunication Network Access to STN |
| NEWS WWW | | | CAS World Wide Web Site (general information) |

Enter NEWS followed by the item number or name to see news on that specific topic.

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* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 10:08:42 ON 26 AUG 2005

=> file reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'REGISTRY' ENTERED AT 10:08:50 ON 26 AUG 2005

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STRUCTURE FILE UPDATES: 24 AUG 2005 HIGHEST RN 861772-82-9

DICTIONARY FILE UPDATES: 24 AUG 2005 HIGHEST RN 861772-82-9

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

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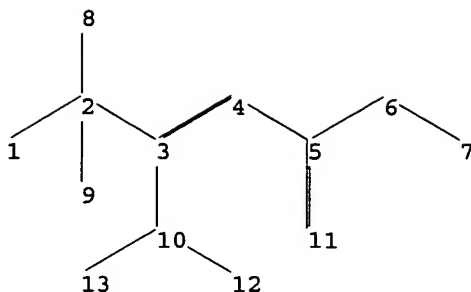
*
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
*

Structure search iteration limits have been increased. See HELP SLIMITS for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>

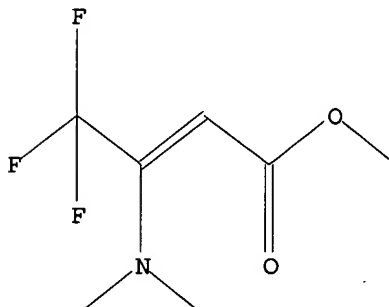
Uploading C:\Documents and Settings\PZucker\My Documents\Examination Auxillary files\10511932\10511932 target cmpd.str



1-2 2-3 2-8 2-9 3-4 4-5

```
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS
10:CLASS 11:CLASS 12:CLASS 13:CLASS
```

| L1 | STR |
|----|-----|
|----|-----|



L2 0 SEA SSS SAM L1

=> search l1 sss sam
SAMPLE SEARCH INITIATED 10:14:43 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 36 TO ITERATE

100.0% PROCESSED 36 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 360 TO 1080
PROJECTED ANSWERS: 0 TO 0

L3 0 SEA SSS SAM L1

=>

=> search l1 sss full
FULL SEARCH INITIATED 10:15:04 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 593 TO ITERATE

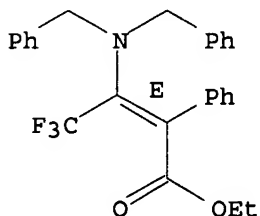
100.0% PROCESSED 593 ITERATIONS 8 ANSWERS
SEARCH TIME: 00.00.01

L4 8 SEA SSS FUL L1

=> d scan

L4 8 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN
IN Benzeneacetic acid, α -[1-[bis(phenylmethyl)amino]-2,2,2-trifluoroethylidene]-, ethyl ester, (α E)- (9CI)
MF C26 H24 F3 N O2

Double bond geometry as shown.

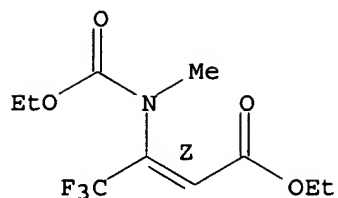


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):8

L4 8 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN
IN 2-Butenoic acid, 3-[(ethoxycarbonyl)methylamino]-4,4,4-trifluoro-, ethyl ester, (2Z)- (9CI)
MF C10 H14 F3 N O4

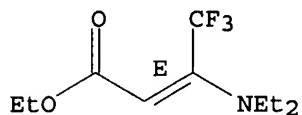
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 8 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN
 IN 2-Butenoic acid, 3-(diethylamino)-4,4,4-trifluoro-, ethyl ester, (2E)-
 (9CI)
 MF C10 H16 F3 N O2

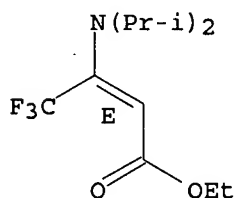
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 8 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN
 IN 2-Butenoic acid, 3-[bis(1-methylethyl)amino]-4,4,4-trifluoro-, ethyl
 ester, (2E)- (9CI)
 MF C12 H20 F3 N O2

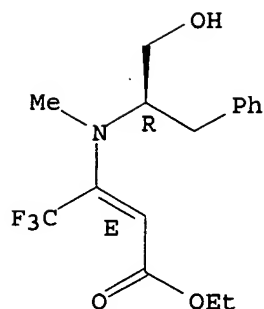
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 8 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN
 IN 2-Butenoic acid, 4,4,4-trifluoro-3-[[[(1R)-1-(hydroxymethyl)-2-
 phenylethyl]methylamino]-, ethyl ester, (2E)- (9CI)
 MF C16 H20 F3 N O3

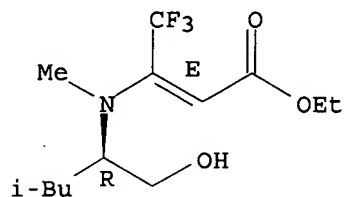
Absolute stereochemistry.
 Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 8 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN
 IN 2-Butenoic acid, 4,4,4-trifluoro-3-[[1R)-1-(hydroxymethyl)-3-methylbutyl]methylamino]-, ethyl ester, (2E)- (9CI)
 MF C13 H22 F3 N O3

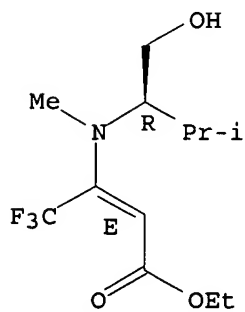
Absolute stereochemistry.
 Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

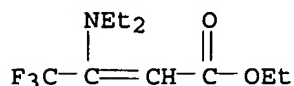
L4 8 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN
 IN 2-Butenoic acid, 4,4,4-trifluoro-3-[[1R)-1-(hydroxymethyl)-2-methylpropyl]methylamino]-, ethyl ester, (2E)- (9CI)
 MF C12 H20 F3 N O3

Absolute stereochemistry.
 Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 8 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN
 IN 2-Butenoic acid, 3-(diethylamino)-4,4,4-trifluoro-, ethyl ester (9CI)
 MF C10 H16 F3 N O2



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> file caplus
 COST IN U.S. DOLLARS
 FULL ESTIMATED COST

| SINCE FILE ENTRY | TOTAL SESSION |
|------------------|---------------|
| 166.06 | 166.27 |

FILE 'CAPLUS' ENTERED AT 10:16:14 ON 26 AUG 2005
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FILE COVERS 1907 - 26 Aug 2005 VOL 143 ISS 10
 FILE LAST UPDATED: 25 Aug 2005 (20050825/ED)

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> l4

L5 5 L4

=> l4/prep

5 L4
 3348673 PREP/RL
 L6 4 L4/PREP
 (L4 (L) PREP/RL)

=> d l6 1-4 ti fbib abs

L6 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2005 ACS on STN
 TI A new synthesis of optically active 3-substituted (3S)-3,4-dihydro-5-(perfluoroalkyl)-2H-[1,4]oxazepin-7-ones
 AN 2003:291077 CAPLUS
 DN 139:117405
 TI A new synthesis of optically active 3-substituted (3S)-3,4-dihydro-5-(perfluoroalkyl)-2H-[1,4]oxazepin-7-ones

AU Richard, Sebastien; Prie, Gildas; Guignard, Alain; Thibonnet, Jerome;
 Parrain, J.-Luc; Duchene, Alain; Abarbri, Mohamed
 CS Laboratoire de Physicochimie des Interfaces et des Milieux Reactionnels,
 Faculte des Sciences de Tours, Tours, F-37200, Fr.
 SO Helvetica Chimica Acta (2003), 86(3), 726-732
 CODEN: HCACAV; ISSN: 0018-019X
 PB Verlag Helvetica Chimica Acta
 DT Journal
 LA English
 OS CASREACT 139:117405
 AB Optically active (perfluoroalkyl)-oxazepin-7-ones were synthesized in two
 steps starting from Et perfluorobut-2-ynoate by direct addition of optically
 active amino alcs. via intermol. Michael addition and lactone formation.
 RE.CNT 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

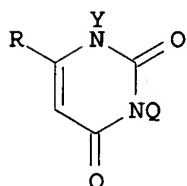
L6 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2005 ACS on STN
 TI Easy synthesis of (E)- or (Z)-perfluorinated β -enaminoesters
 AN 2002:732461 CAPLUS
 DN 138:187392
 TI Easy synthesis of (E)- or (Z)-perfluorinated β -enaminoesters
 AU Prie, Gildas; Richard, Sebastien; Parrain, Jean-Luc; Duchene, Alain;
 Abarbri, Mohamed
 CS Faculte des Sciences de Tours, Laboratoire de Physicochimie des Interfaces
 et des Milieux Reactionnels, Tours, 37200, Fr.
 SO Journal of Fluorine Chemistry (2002), 117(1), 35-41
 CODEN: JFLCAR; ISSN: 0022-1139
 PB Elsevier Science B.V.
 DT Journal
 LA English
 OS CASREACT 138:187392
 GI



AB (E)- or (Z)-perfluorinated β -enaminoesters, e.g. I and II, were
 prepared by direct addition of primary or secondary amines to Et
 perfluoroalkynoates without any catalyst.
 RE.CNT 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2005 ACS on STN
 TI Preparation of 6-(perfluoroalkyl)uracils from 3-(alkoxycarbonylamino)-3-
 perfluoroalkylacrylates and amines.
 AN 2000:592705 CAPLUS
 DN 133:177187
 TI Preparation of 6-(perfluoroalkyl)uracils from 3-(alkoxycarbonylamino)-3-
 perfluoroalkylacrylates and amines.
 IN Kameswaran, Venkataraman
 PA American Cyanamid Company, USA
 SO PCT Int. Appl., 91 pp.
 CODEN: PIXXD2
 DT Patent
 LA English
 FAN.CNT 1
 PATENT NO. KIND DATE APPLICATION NO. DATE

| | | | | | |
|----|--|--|----------|-----------------|------------|
| PI | WO 2000049003 | A1 | 20000824 | WO 2000-US3795 | 20000214 |
| | W: | AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | |
| | RW: | GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | | | |
| | CA 2362996 | AA | 20000824 | US 1999-250725 | A 19990216 |
| | | | | CA 2000-2362996 | 20000214 |
| | | | | US 1999-250725 | A 19990216 |
| | | | | WO 2000-US3795 | W 20000214 |
| | EP 1150962 | A1 | 20011107 | EP 2000-911810 | 20000214 |
| | EP 1150962 | B1 | 20040428 | | |
| | R: | AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO | | | |
| | | | | US 1999-250725 | A 19990216 |
| | | | | WO 2000-US3795 | W 20000214 |
| | BR 2000008306 | A | 20020122 | BR 2000-8306 | 20000214 |
| | | | | US 1999-250725 | A 19990216 |
| | | | | WO 2000-US3795 | W 20000214 |
| | JP 2002537290 | T2 | 20021105 | JP 2000-599743 | 20000214 |
| | | | | US 1999-250725 | A 19990216 |
| | | | | WO 2000-US3795 | W 20000214 |
| | AT 265440 | E | 20040515 | AT 2000-911810 | 20000214 |
| | | | | US 1999-250725 | A 19990216 |
| | | | | WO 2000-US3795 | W 20000214 |
| OS | CASREACT 133:177187; MARPAT 133:177187 | | | | |
| GI | | | | | |



I

AB Title compds. [I; R = CnF2n+1; n = 1-6; Y = H, alkyl; Q = alkyl, (substituted) Ph, PhCH2, heteroaryl, methyleneheteroaryl], were prepared by reaction of CnF2n+1C(:CHCO2Z1)N(Y)CO2Z [Z, Z1 = alkyl, (substituted) PhCH2; n, Y as above] with QNH2 in the presence of base followed by optional alkylation. Thus, Et [(ethoxycarbonyl)amino]-4,4,4-trifluorocrotonate (preparation given), Me2CHNH2, and DBU were refluxed in xylene to give 61% 3-isopropyl-6-trifluoromethyl-2,4-(1H,3H)-pyrimidinedione.

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2005 ACS on STN

TI Concise stereoselective synthesis of 1-perfluoroalkyl enamines via the addition of N-lithiated amines to enol ethers and their subsequent metalation to form new functionalized enamines

AN 1998:317130 CAPLUS

DN 129:95082

TI Concise stereoselective synthesis of 1-perfluoroalkyl enamines via the addition of N-lithiated amines to enol ethers and their subsequent metalation to form new functionalized enamines

AU Begue, Jean-Pierre; Bonnet-Delpon, Daniele; Bouvet, Denis; Rock, Michael

H.
 CS Centre d'Etudes Pharmaceutiques, BioCIS-CNRS, Chatenay-Malabry, F-92296, Fr.
 SO Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1998), (11), 1797-1800
 CODEN: JCPRB4; ISSN: 0300-922X
 PB Royal Society of Chemistry
 DT Journal
 LA English
 OS CASREACT 129:95082
 AB Addition of lithium amides, e.g., (PhCH₂)₂NLi, derived from a range of cyclic, sterically demanding, and chiral amines, to trifluoromethyl (Z)-enol ethers, e.g., (Z)-F₃CC(OEt):CHPh and (Z)-F₃CC(OEt):CHC₆H₄OMe-4, gave stereoselectively the corresponding (Z)-enamines, e.g. (Z)-(PhCH₂)₂NC(CF₃):CHPh and (Z)-(PhCH₂)₂NC(CF₃):CHC₆H₄OMe-4, in good yields. The reaction was extended to perfluoroalkyl and chlorofluoroalkyl enol ethers, e.g., EtOC(CClF₂):CHPh. The enamines react with Me₃CLi to give vinylic anions and, after quenching with aldehydes and Et chloroformate, provide new functionalized enamines, e.g., (PhCH₂)₂NC(CF₃):C(Ph)CH(OH)Et.
 RE.CNT 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> trifluoroacetate
 8419 TRIFLUOROACETATE
 818 TRIFLUOROACETATES
 L7 8790 TRIFLUOROACETATE
 (TRIFLUOROACETATE OR TRIFLUOROACETATES)

=> 16 and 17
 L8 0 L6 AND L7

=> FIL CASREACT

| | | |
|--|------------|---------|
| COST IN U.S. DOLLARS | SINCE FILE | TOTAL |
| | ENTRY | SESSION |
| FULL ESTIMATED COST | 17.98 | 184.25 |
| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE | TOTAL |
| | ENTRY | SESSION |
| CA SUBSCRIBER PRICE | -2.92 | -2.92 |

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FILE CONTENT:1840 - 21 Aug 2005 VOL 143 ISS 8

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```

*****
*
*   CASREACT now has more than 9.2 million reactions
*
*****

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> SET NOTICE DISPLAY 1

NOTICE SET TO 1 U.S. DOLLAR FOR DISPLAY COMMAND
SET COMMAND COMPLETED

=> D ACC 138:187392 ALL

THE ESTIMATED COST FOR THIS REQUEST IS 6.62 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N:n
REQUEST CANCELED

=> SET NOTICE LOGIN DISPLAY

NOTICE SET TO OFF FOR DISPLAY COMMAND
SET COMMAND COMPLETED

=> logoff hold

| | | |
|--|------------------|---------------|
| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
| FULL ESTIMATED COST | 0.43 | 184.68 |
| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION |
| CA SUBSCRIBER PRICE | 0.00 | -2.92 |

SESSION WILL BE HELD FOR 60 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 10:21:26 ON 26 AUG 2005

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSSPTA1623PAZ

PASSWORD:

* * * * * RECONNECTED TO STN INTERNATIONAL * * * * *
SESSION RESUMED IN FILE 'CASREACT' AT 10:55:30 ON 26 AUG 2005
FILE 'CASREACT' ENTERED AT 10:55:30 ON 26 AUG 2005
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| | | |
|--|------------------|---------------|
| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
| FULL ESTIMATED COST | 0.43 | 184.68 |
| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION |
| CA SUBSCRIBER PRICE | 0.00 | -2.92 |

=> logoff hold

| | | |
|--|------------------|---------------|
| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
| FULL ESTIMATED COST | 0.43 | 184.68 |
| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION |
| CA SUBSCRIBER PRICE | 0.00 | -2.92 |

SESSION WILL BE HELD FOR 60 MINUTES

STN INTERNATIONAL SESSION SUSPENDED AT 10:55:43 ON 26 AUG 2005

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSSPTA1623PAZ

PASSWORD:

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SESSION RESUMED IN FILE 'CASREACT' AT 11:22:56 ON 26 AUG 2005
FILE 'CASREACT' ENTERED AT 11:22:56 ON 26 AUG 2005
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| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
|----------------------|------------------|---------------|
| FULL ESTIMATED COST | 0.43 | 184.68 |

| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION |
|--|------------------|---------------|
| CA SUBSCRIBER PRICE | 0.00 | -2.92 |

=> file reg

| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
|----------------------|------------------|---------------|
| FULL ESTIMATED COST | 0.43 | 184.68 |

| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION |
|--|------------------|---------------|
| CA SUBSCRIBER PRICE | 0.00 | -2.92 |

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STRUCTURE FILE UPDATES: 24 AUG 2005 HIGHEST RN 861772-82-9
DICTIONARY FILE UPDATES: 24 AUG 2005 HIGHEST RN 861772-82-9

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TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

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*
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
*

Structure search iteration limits have been increased. See HELP SLIMITS for details.

Experimental and calculated property data are now available. For more

information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=> e ethyl-4,4,4-trifluoroacetoacetate/cn

| | | |
|-----|-------|---|
| E1 | 1 | ETHYL-3-PROPOXYBENZIMIDATE/CN |
| E2 | 1 | ETHYL-4,12-TRIDECADIENOATE/CN |
| E3 | 0 --> | ETHYL-4,4,4-TRIFLUOROACETOACETATE/CN |
| E4 | 1 | ETHYL-4,6-DI-O-ACETYL-A-Ψ-D-GLUCAL/CN |
| E5 | 1 | ETHYL-4,6-DI-O-ACETYL-2,3-DIDEOXY-A-D-ERYTHROHEX-2-ENO PYRANOSIDE/CN |
| E6 | 1 | ETHYL-4-(9-(1-ETHYL-4(1H)-QUINOLYLIDENE)-5-HYDROXY-1,3,5,7-N ONATETRAENYL)-1-QUINOLINIUM PERCHLORATE, ACETATE/CN |
| E7 | 1 | ETHYL-4-ACETYL-3,5-DIMETHYLPYRROLE-2-CARBOXYLATE/CN |
| E8 | 1 | ETHYL-4-BROMO-2,5-DICHLOROPHENYL PHOSPHOROTHIONATE/CN |
| E9 | 1 | ETHYL-4-GUANIDINO BENZOATE/CN |
| E10 | 1 | ETHYL-4-METHYLDIBENZOTHIOPHENE/CN |
| E11 | 1 | ETHYL-4H-1,2,4-TRIAZOLE-4-CARBAMATE/CN |
| E12 | 1 | ETHYL-6-AMINO-3,4-DIISOBUTOXYBENZOATE/CN |

=> e ethyl-4,4,4-trifluoroacetoacetate/cn

| | | |
|-----|-------|---|
| E1 | 1 | ETHYL-3-PROPOXYBENZIMIDATE/CN |
| E2 | 1 | ETHYL-4,12-TRIDECADIENOATE/CN |
| E3 | 0 --> | ETHYL-4,4,4-TRIFLUOROACETOACETATE/CN |
| E4 | 1 | ETHYL-4,6-DI-O-ACETYL-A-Ψ-D-GLUCAL/CN |
| E5 | 1 | ETHYL-4,6-DI-O-ACETYL-2,3-DIDEOXY-A-D-ERYTHROHEX-2-ENO PYRANOSIDE/CN |
| E6 | 1 | ETHYL-4-(9-(1-ETHYL-4(1H)-QUINOLYLIDENE)-5-HYDROXY-1,3,5,7-N ONATETRAENYL)-1-QUINOLINIUM PERCHLORATE, ACETATE/CN |
| E7 | 1 | ETHYL-4-ACETYL-3,5-DIMETHYLPYRROLE-2-CARBOXYLATE/CN |
| E8 | 1 | ETHYL-4-BROMO-2,5-DICHLOROPHENYL PHOSPHOROTHIONATE/CN |
| E9 | 1 | ETHYL-4-GUANIDINO BENZOATE/CN |
| E10 | 1 | ETHYL-4-METHYLDIBENZOTHIOPHENE/CN |
| E11 | 1 | ETHYL-4H-1,2,4-TRIAZOLE-4-CARBAMATE/CN |
| E12 | 1 | ETHYL-6-AMINO-3,4-DIISOBUTOXYBENZOATE/CN |

=> e ethyl 4,4,4-trifluoroacetoacetate/cn

| | | |
|-----|-------|---|
| E1 | 1 | ETHYL 4,4,4-TRIFLUORO-3-OXOBUTANOATE/CN |
| E2 | 1 | ETHYL 4,4,4-TRIFLUORO-3-OXOBUTYRATE/CN |
| E3 | 1 --> | ETHYL 4,4,4-TRIFLUOROACETOACETATE/CN |
| E4 | 1 | ETHYL 4,4,4-TRIFLUOROACETYLACETONATE/CN |
| E5 | 1 | ETHYL 4,4,4-TRIFLUOROBUTANOATE/CN |
| E6 | 1 | ETHYL 4,4,4-TRIFLUOROBUTYRATE/CN |
| E7 | 1 | ETHYL 4,4,4-TRIFLUOROCROTONATE/CN |
| E8 | 1 | ETHYL 4,4,4-TRINITROBUTYRATE/CN |
| E9 | 1 | ETHYL 4,4,5,5,5-PENTAFLUORO-3-METHOXY-2-PENTENOATE/CN |
| E10 | 1 | ETHYL 4,4,5,5,5-PENTAFLUORO-3-OXOPENTANOATE/CN |
| E11 | 1 | ETHYL 4,4,5,5,5-PENTAFLUORO-3-OXOVALERATE/CN |
| E12 | 1 | ETHYL 4,4,5,5-TETRAFLUORO-3-OXOPENTANOATE/CN |

=> e3

L9 1 "ETHYL 4,4,4-TRIFLUOROACETOACETATE"/CN

=> d 19

L9 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2005 ACS on STN

RN 372-31-6 REGISTRY

ED Entered STN: 16 Nov 1984

CN Butanoic acid, 4,4,4-trifluoro-3-oxo-, ethyl ester (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Acetoacetic acid, 4,4,4-trifluoro-, ethyl ester (6CI, 8CI)

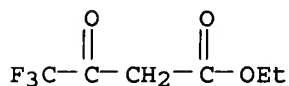
OTHER NAMES:

CN 1-Ethoxy-4,4,4-trifluorobutane-1,3-dione

CN 4,4,4-Trifluoro-3-oxobutanoic acid ethyl ester

CN 4,4,4-Trifluoroacetoacetic acid ethyl ester

CN Ethyl (trifluoroacetyl)acetate
 CN Ethyl γ,γ,γ -trifluoroacetoacetate
 CN Ethyl ω,ω,ω -trifluoroacetoacetate
 CN Ethyl 3-oxo-4,4,4-trifluorobutanoate
 CN Ethyl 4,4,4-trifluoro-3-oxobutanoate
 CN Ethyl 4,4,4-trifluoro-3-oxobutyrate
 CN **Ethyl 4,4,4-trifluoroacetoacetate**
 CN Ethyl 4,4,4-trifluoroacetylacetonate
 CN Ethyl trifluoroacetoacetate
 CN NSC 42739
 CN NSC 49750
 FS 3D CONCORD
 MF C6 H7 F3 O3
 CI COM
 LC STN Files: AGRICOLA, BEILSTEIN*, BIOBUSINESS, BIOSIS, CA, CAOLD, CAPLUS,
 CASREACT, CBNB, CHEMCATS, CHEMINFORMRX, CHEMLIST, CSCHM, GMELIN*,
 HODOC*, IFICDB, IFIPAT, IFIUDB, PS, SPECINFO, SYNTHLINE, TOXCENTER,
 USPAT2, USPATFULL
 (*File contains numerically searchable property data)
 Other Sources: EINECS**, NDSL**, TSCA**
 (**Enter CHEMLIST File for up-to-date regulatory information)



****PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT****

616 REFERENCES IN FILE CA (1907 TO DATE)
 9 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
 616 REFERENCES IN FILE CAPLUS (1907 TO DATE)
 25 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=> file caplus

| | | |
|--|------------------|---------------|
| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
| FULL ESTIMATED COST | 7.73 | 192.41 |
| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION |
| CA SUBSCRIBER PRICE | 0.00 | -2.92 |

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FILE COVERS 1907 - 26 Aug 2005 VOL 143 ISS 10
 FILE LAST UPDATED: 25 Aug 2005 (20050825/ED)

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> l9/prep

616 L9
3348673 PREP/RL
L10 26 L9/PREP
(L9 (L) PREP/RL)

=> alkoxide

18843 ALKOXIDE
14664 ALKOXIDES
L11 26898 ALKOXIDE
(ALKOXIDE OR ALKOXIDES)

=> l10 and l11

L12 0 L10 AND L11

=> ?oxide

L13 2564126 ?OXIDE

=> l10 and l12

L14 0 L10 AND L12

=> claiasen

0 CLAIASEN
L15 0 CLAIASEN

=> claisen

6500 CLAISEN
3 CLAISENS
L16 6502 CLAISEN
(CLAISEN OR CLAISENS)

=> l10 and l16

L17 3 L10 AND L16

=> d l17 1-3 ti fbib abs

L17 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN

TI Manufacture of alkyl trifluoroacetoacetate

AN 1988:612818 CAPLUS

DN 109:212818

TI Manufacture of alkyl trifluoroacetoacetate

IN Mysinsky, Edward

PA Monsanto Co., Japan

SO Jpn. Kokai Tokkyo Koho, 8 pp.

CODEN: JKXXAF

DT Patent

LA Japanese

FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|----|-------------|------|----------|-----------------|----------|
| PI | JP 63156753 | A2 | 19880629 | JP 1986-298587 | 19861215 |
| | JP 05029344 | B4 | 19930430 | | |
| | | | | JP 1986-298587 | 19861215 |

AB The title compds. are prepared by reacting C1-5 alkyl 3-alkoxy-3-hydroxy-4,4,4-trifluorobutanoate (I) with acetyl halide or Ac2O under pressure at a temperature $\geq 10^\circ$ but lower than the reflux temperature of the reaction mixture Adding 79.0 parts Et trifluoroacetate to 61.8 parts cyclohexane (II) and 22.3 parts NaOH (as 60% mineral oil dispersion), heating with 53.9 parts EtOAc for 2 h at 45-60°, diluting with 55.7 parts II, neutralizing with HCl, refluxing the slurry with 41.5 parts CH3COCl,

filtering, washing and distilling provided 75% Et trifluoroacetoacetate.

L17 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN

TI Preparation of alkyl trifluoroacetoacetate

AN 1987:439216 CAPLUS

DN 107:39216

TI Preparation of alkyl trifluoroacetoacetate

IN Micinski, Edward

PA Monsanto Co. , USA

SO U.S., 6 pp.

CODEN: USXXAM

DT Patent

LA English

FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|----|---|------|----------|-----------------|------------|
| PI | US 4647689 | A | 19870303 | US 1982-403754 | 19820730 |
| | CA 1284153 | A1 | 19910514 | CA 1986-524197 | 19861201 |
| | | | | US 1982-403754 | 19820730 |
| | AU 591536 | B2 | 19891207 | AU 1986-66060 | 19861203 |
| | AU 8666060 | A1 | 19880609 | | |
| | | | | US 1982-403754 | 19820730 |
| | EP 270724 | A1 | 19880615 | EP 1986-870187 | 19861212 |
| | EP 270724 | B1 | 19901128 | | |
| | R: AT, BE, CH, DE, ES, FR, GB, IT, LI, LU, NL, SE | | | | |
| | | | | US 1982-403754 | 19820730 |
| | AT 58719 | E | 19901215 | AT 1986-870187 | 19861212 |
| | | | | EP 1986-870187 | A 19861212 |

OS CASREACT 107:39216

AB The title C1-5 alkyl trifluoroacetoacetates (I) are prepared by acetylation of C1-5 alkyl 3-alkoxy-3-hydroxy-4,4,4-trifluorobutanoate obtained from **Claisen** condensation of alkyl trifluoroacetate and alkyl acetate in the presence of a strong base. F3CCO2Et was condensed with EtOAc in the presence of NaH to give a mixture containing EtOH and F3COCH2CO2Et.Na, which

was

neutralized with HCl to give F3CC(OH)(OEt)CH2CO2Et, treatment of which with AcCl gave 75% F3CCOCH2COEt.

L17 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN

TI Synthesis and spectral study of 4-(perfluoroalkyl)coumarins

AN 1982:544728 CAPLUS

DN 97:144728

TI Synthesis and spectral study of 4-(perfluoroalkyl)coumarins

AU Bayer, V.; Pastor, R.; Cambon, A.

CS Fac. Sci., Unites Enseign. Rech., Nice, 06034, Fr.

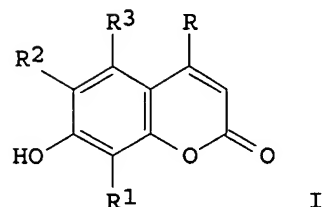
SO Journal of Fluorine Chemistry (1982), 20(2), 187-202

CODEN: JFLCAR; ISSN: 0022-1139

DT Journal

LA French

GI



AB Coumarins I [R = (CF₂)_nCF₃ (n = 0, 2, 4, 6); R₁ = H, OH, Me; R₂, R₃ = H, OH] were obtained by treating RCOCH₂CO₂Et with phenols. RCOCH₂CO₂Et were prepared by Claisen condensation of RCO₂Et with EtOAc. The ¹H and ¹⁹F-NMR spectra of I are discussed. A new long distance H-F coupling constant [5J] was observed and interpreted as a coupling through space.

=> logoff hold

| | | |
|--|------------|---------|
| COST IN U.S. DOLLARS | SINCE FILE | TOTAL |
| | ENTRY | SESSION |
| FULL ESTIMATED COST | 21.45 | 213.86 |
| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE | TOTAL |
| | ENTRY | SESSION |
| CA SUBSCRIBER PRICE | -2.19 | -5.11 |

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STN INTERNATIONAL SESSION SUSPENDED AT 11:30:10 ON 26 AUG 2005

Connecting via Winsock to STN

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LOGINID:SSSPTA1623PAZ

PASSWORD:

* * * * * RECONNECTED TO STN INTERNATIONAL * * * * *
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FILE 'CAPLUS' ENTERED AT 12:22:09 ON 26 AUG 2005
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|--|------------|---------|
| COST IN U.S. DOLLARS | SINCE FILE | TOTAL |
| | ENTRY | SESSION |
| FULL ESTIMATED COST | 21.45 | 213.86 |
| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE | TOTAL |
| | ENTRY | SESSION |
| CA SUBSCRIBER PRICE | -2.19 | -5.11 |

=> d his

(FILE 'HOME' ENTERED AT 10:08:42 ON 26 AUG 2005)

FILE 'REGISTRY' ENTERED AT 10:08:50 ON 26 AUG 2005

L1 STRUCTURE UPLOADED
L2 0 SEARCH L1 SSS SAM
L3 0 SEARCH L1 SSS SAM
L4 8 SEARCH L1 SSS FULL

FILE 'CAPLUS' ENTERED AT 10:16:14 ON 26 AUG 2005

L5 5 L4
L6 4 L4/PREP
L7 8790 TRIFLUOROACETATE
L8 0 L6 AND L7

FILE 'CASREACT' ENTERED AT 10:21:01 ON 26 AUG 2005

SET NOTICE DISPLAY 1
SET NOTICE LOGIN DISPLAY

FILE 'REGISTRY' ENTERED AT 11:23:02 ON 26 AUG 2005

E ETHYL-4,4,4-TRIFLUOROACETOACETATE/CN
E ETHYL-4,4,4-TRIFLUOROACETOACETATE/CN

E ETHYL 4,4,4-TRIFLUOROACETOACETATE/CN

L9 1 E3

FILE 'CAPLUS' ENTERED AT 11:25:03 ON 26 AUG 2005

L10 26 L9/PREP
L11 26898 ALKOXIDE
L12 0 L10 AND L11
L13 2564126 ?OXIDE
L14 0 L10 AND L12
L15 0 CLAIASEN
L16 6502 CLAISEN
L17 3 L10 AND L16

=> logoff hold

COST IN U.S. DOLLARS

| SINCE FILE | TOTAL |
|------------|---------|
| ENTRY | SESSION |
| 21.90 | 214.31 |

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

| SINCE FILE | TOTAL |
|------------|---------|
| ENTRY | SESSION |
| -2.19 | -5.11 |

CA SUBSCRIBER PRICE

SESSION WILL BE HELD FOR 60 MINUTES

STN INTERNATIONAL SESSION SUSPENDED AT 12:22:27 ON 26 AUG 2005